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Potential Curves and Rotational Perturbations of CN

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# POTENTIAL CURVES AND ROTATIONAL PERTURBATIONS OF CN\*

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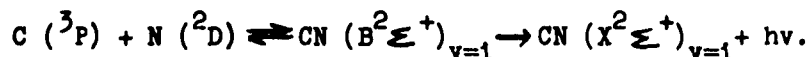
## ABSTRACT

Potential energy curves for the  $X^2\Sigma^+$ ,  $A^2\Pi_{3/2}$ ,  $A^2\Pi_{1/2}$ ,  $B^2\Sigma^+$ ,  $D^2\Pi_1$  and  $J^2\Delta_1$  states of CN have been calculated from the experimental data by the Rydberg-Klein-Rees method. The resulting curves have been used to discuss qualitatively the rotational perturbations in the  $v = 7$  vibrational level of the  $^2\Pi_{3/2}$  electronic state.

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## INTRODUCTION

This is one of a series of papers dealing with the potential energy curves of diatomic species which are of interest in the study of flames and astrophysical problems. The species CN is present in hot flames,<sup>1</sup> in solar and stellar atmospheres,<sup>2</sup> and in the heads of comets.<sup>2</sup> In addition, the band spectra of CN is observed when air and hydrocarbon impurities are present in a shocked gas.<sup>3</sup> The following reactions have been proposed as possible causes for CN emission in shocks.<sup>3,4</sup>



Carbon atoms are known to exist in hot flames<sup>5</sup> and it is therefore possible that the above atom recombination reaction is also of importance in these systems. For these reasons it was thought that a reliable knowledge of the potential curves for CN would be of some value.

The rotational perturbations observed in the  $\text{A}^2\Pi_{3/2}$  and  $\text{X}^2\Sigma$  states of CN are also of interest.<sup>6</sup> These two curves cross at an energy near those of the perturbed levels. Hence if one has reliable potential curves for these states, then one should be able to discuss qualitatively the effects of the Franck-Condon factor in the perturbations along the lines given by Mulliken.<sup>7</sup>

Spectroscopic data<sup>6,8,9</sup> are available to some extent on the  $\text{X}^2\Sigma^+$ ,  $\text{A}^2\Pi_1$ ,  $\text{B}^2\Sigma^+$ ,  $\text{D}^2\Pi_1$ , and  $\text{J}^2\Delta_1$  electronic states of CN. The Rydberg-Klein-Rees (RKR) method<sup>10</sup> therefore offers a simple and reliable procedure to obtain potential curves for these five electronic states.

## PROCEDURE AND RESULTS

The RKR method is a WKB approximation which allows one to obtain reliable potential curves from the measured vibrational and rotational levels of a diatomic molecule. The method and procedure have been described in detail elsewhere<sup>10,11</sup> and are not repeated here. The method yields the maximum and minimum points of vibration,  $r_{\max}$  and  $r_{\min}$ , at a given energy,  $U$ . The method is, of course, limited to regions of energy for which the necessary spectroscopic data are available. The results for the  $X^2\Sigma^+$ ,  $A^2\Pi_{3/2}$ ,  $A^2\Pi_{1/2}$ ,  $B^2\Sigma^+$ ,  $D^2\Pi_1$  and  $J^2\Delta_1$  electronic states of CN are given in Table I and corresponding curves are shown in Fig. 1. The  $A^2\Pi_1$  electronic states are intermediate between Hund's cases (a) and (b) and hence the  $^2\Pi_{3/2}$  and  $^2\Pi_{1/2}$  states were calculated from a modified RKR procedure.<sup>12</sup> The number of significant figures given for the  $X^2\Sigma$  and  $A^2\Pi_1$  states is one more than is usually given. We have done this so as to give a more precise discussion of the rotational perturbations in these two states. It must be remembered however, that there is some uncertainty in the last figure given.

## ROTATIONAL PERTURBATIONS

The rotational perturbations observed in the  $A^2\Pi_{3/2}$  and the  $X^2\Sigma^+$  states of CN have been discussed in detail by Herzberg<sup>2</sup> and by Jenkins, Roots, and Mulliken.<sup>7</sup> The latter authors have pointed out that the rotational perturbations occur in the  $v = 11$  vibrational level of the  $^2\Sigma^+$  and the  $v = 7$  (see Herzberg, ref.2) level of the  $^2\Pi_{3/2}$  state. The maximum perturbations occur near values of  $J = 12 \frac{1}{2}$  and  $13 \frac{1}{2}$ . The perturbations are due to the fact that the vibrational-rotational levels of both states have almost the

same energies for these values of  $J$  and also that the effective potential energies, given by

$$U_{\text{eff}} = U(r) + E_{\text{rot}}(r) \quad (1)$$

where  $U(r)$  is the potential for the rotationless state, cross at these energies. The general situation is illustrated in Fig. 2.

With our present more precise knowledge of the potential curves, it should be possible to look at the details of the crossing more precisely. To do this, one has to first calculate the effective potential curves for the two states for the  $J$  values of interest. This can be done from equation (1) with the appropriate expression for  $E_{\text{rot}}$ . For the  $X^1\Sigma^+$  state which falls in Hund's case (b) the rotational energy is given simply by

$$E_{\text{rot}}(r) = \frac{h^2}{8\pi^2 \mu r^2} N(N+1) \quad (2)$$

where  $N$  is the quantum number associated with the sum of orbital electronic angular momentum and the angular momentum of the nuclei. The  $A^2\Pi_{3/2}$  electronic state is an example of a state intermediate between Hund's cases (a) and (b) and hence we have taken the rotational energy to be given by <sup>13,12</sup>

$$E_{\text{rot}}(r) = B_r \left[ (J + 1/2)^2 - \Lambda^2 - \frac{1}{2} \sqrt{4(J + \frac{1}{2})^2 + Y_r(Y_r - 4)\Lambda^2} \right] \quad (3)$$

since the  $A^2\Pi_1$  is an inverted doublet. In this expression  $Y_r = A_r/B_r$ ,  $B_r = h^2/8\pi^2 \mu r^2$ ,  $A_r$  is the spin-axis coupling constant<sup>2</sup> and  $J = N + 1/2$ . In this calculation,  $A_r$  has been taken to be a constant independent of  $r$  since  $A$  was found to be independent of the vibrational levels.<sup>6</sup> (This is only a

plausible reason that  $A_r$  can be independent of  $r$ ). The values of  $U(r)$  were taken from Table I.

The results for the different  $J$  values of interest can best be summarized in tabular form. These are given in Table II and the appropriate definition of the various quantities are illustrated in Fig. 3. There are several things of interest about the results. For one thing, the rotational levels of the  $v = 7$  level of the  $A^2\Pi_{3/2}$  state are quite close to the energy at which the effective potential energy curves cross for values of  $J$  from  $10\frac{1}{2}$  to  $18\frac{1}{2}$ . For  $J \geq 12\frac{1}{2}$ , the crossing points and the  $r'$  and  $r''$  distances are within  $0.001\text{ \AA}$ , the expected error in the RKR method. However a small difference in  $r'$  and  $r''$  can cause a relatively large difference in  $E_x - E(^2\Pi_{3/2})(v=7, J)$  since the  $A^2\Pi_{3/2}$  and  $X^2\Sigma^+$  curves have almost the same slope in this region. We can conclude therefore that the  $r', r''$  and  $r_x$  distances are extremely close to one another and that the energies of crossing  $E_x$ , are not appreciably different from the rotational energies of the  $^2\Pi_{3/2}$  and  $^2\Sigma^+$  states for the range of  $J$  values considered. Finally we notice that the difference in the energy levels of the two states changes in sign as  $J$  varies from  $10\frac{1}{2}$  to  $18\frac{1}{2}$  and is almost zero for  $J = 12\frac{1}{2}, 13\frac{1}{2}$ , and  $14\frac{1}{2}$ .<sup>6</sup> The probability of perturbation is proportional to an electronic rotation factor and to a Franck-Condon factor<sup>7</sup>

$$\int \chi_A^{Jv}(r) \chi_B^{Jv}(r) dr \quad (4)$$



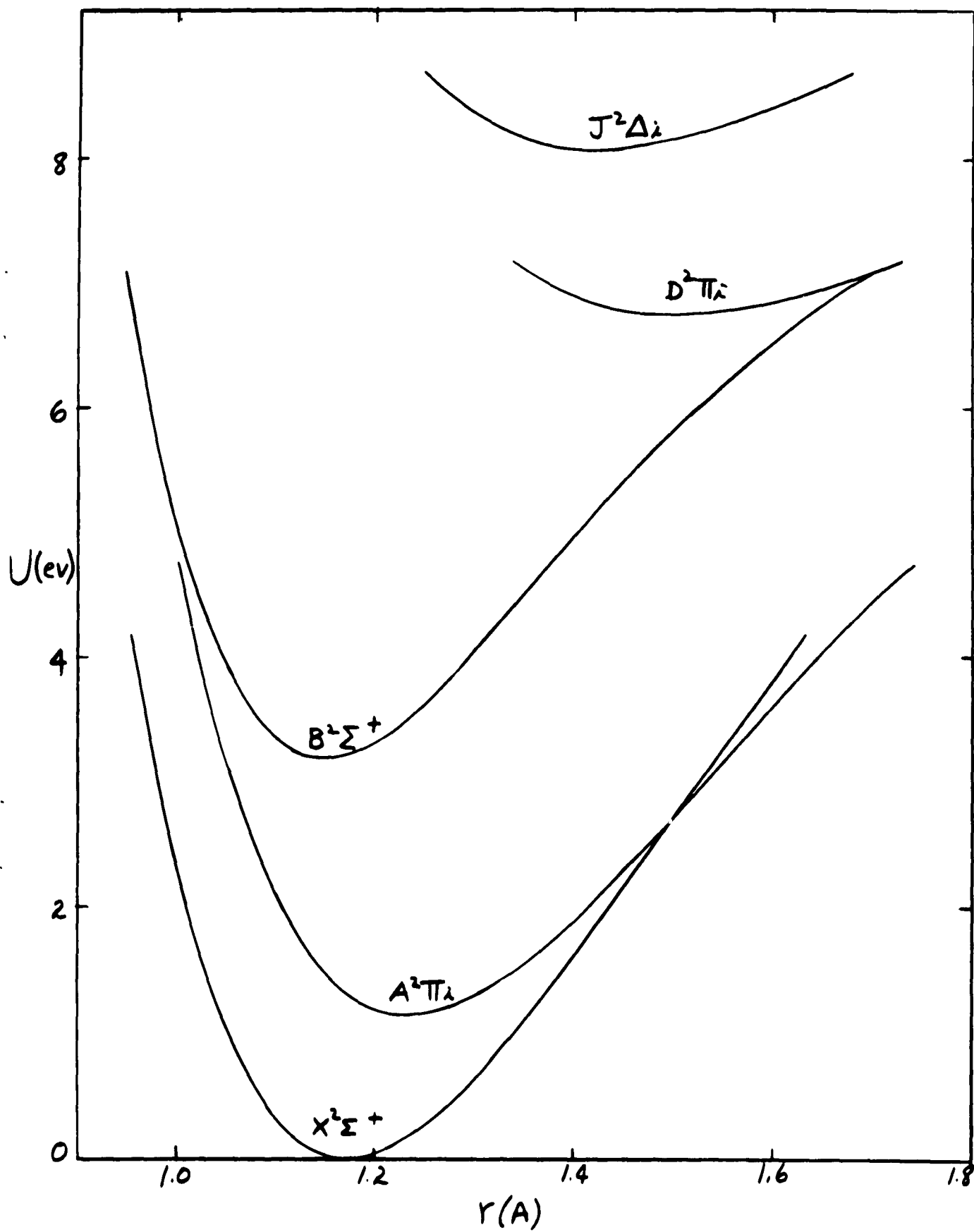
where  $\psi_A^{Jv}$  is the vibrational-rotational wave function of state A and  $\psi_B^{Jv}$  is the corresponding wave function for state B. The Franck-Condon factor depends on the relative position and forms of the potential curves. In the cases under consideration here, the overlap integral (4) should be quite large for  $J = 10 \frac{1}{2}$  to  $18 \frac{1}{2}$ . This is because the energy of the vibrational-rotational levels are close together and also because the turning-points of the motion in the corresponding states are almost identical to within the error of the graphical method and the RKR results. Both factors contribute to large overlap. Hence, according to the Franck-Condon factor alone, the perturbations should be large and extensive. In the case of a heterogeneous predissociation considered here,<sup>7</sup> the electronic rotation factor is nearly a constant times  $J(J + 1)$ . The constant depends on the nature of the two interacting states. In the present case, it must be small to offset the rather large expected Franck-Condon factor. These conclusions agree with those obtained by Mulliken over thirty years ago on the basis of simple Morse curves which can be regarded as giving only rough approximations to the actual curves in the regions of interest here.

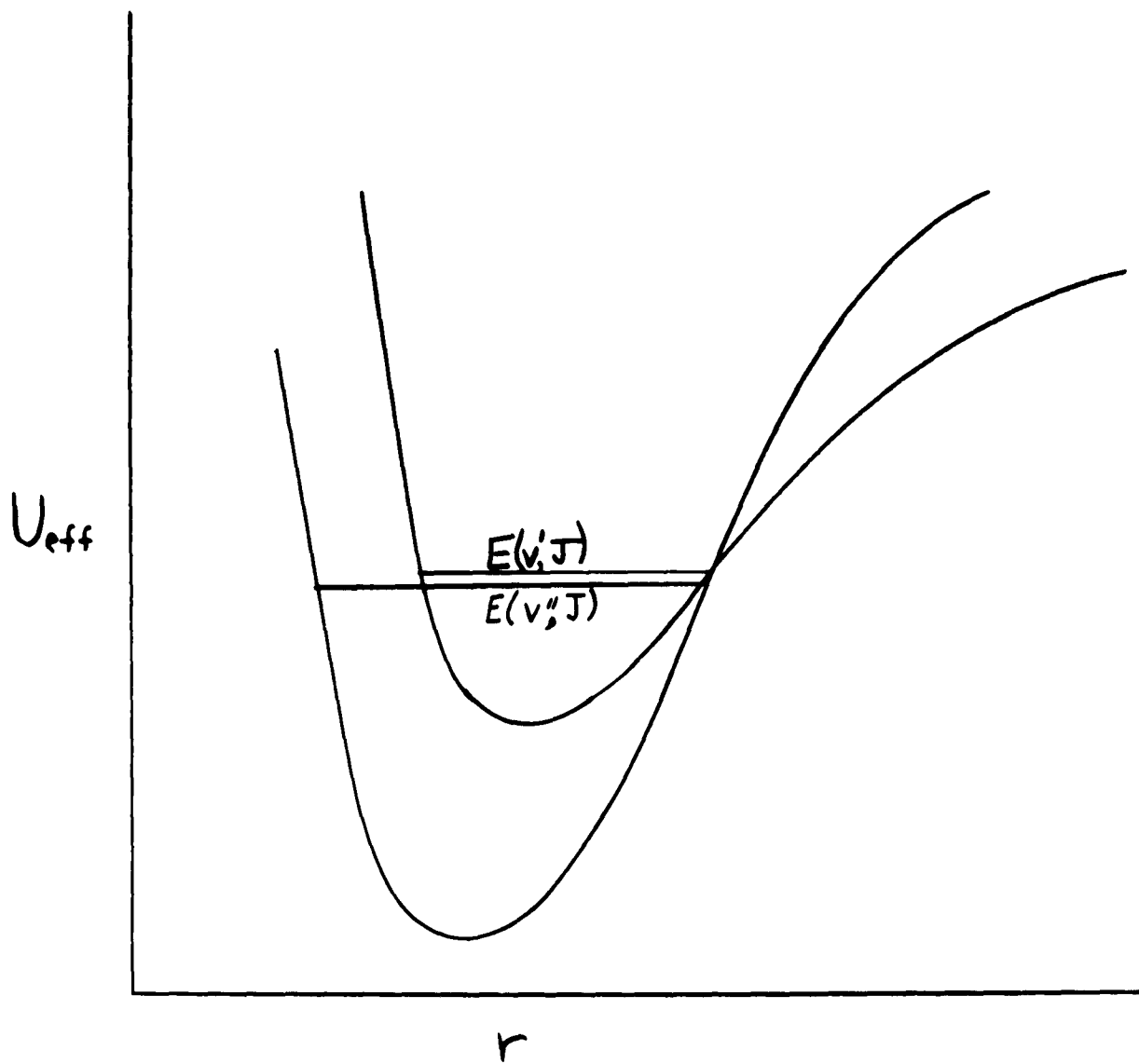
Figure Captions

Fig. 1. Potential Energy Curves for various states of CN

Fig. 2. Illustration of the crossing of effective potential curves and how it affects perturbations (see text).

Fig. 3. Diagram to illustrate the important energy and distance values in the discussion of rotational perturbations.





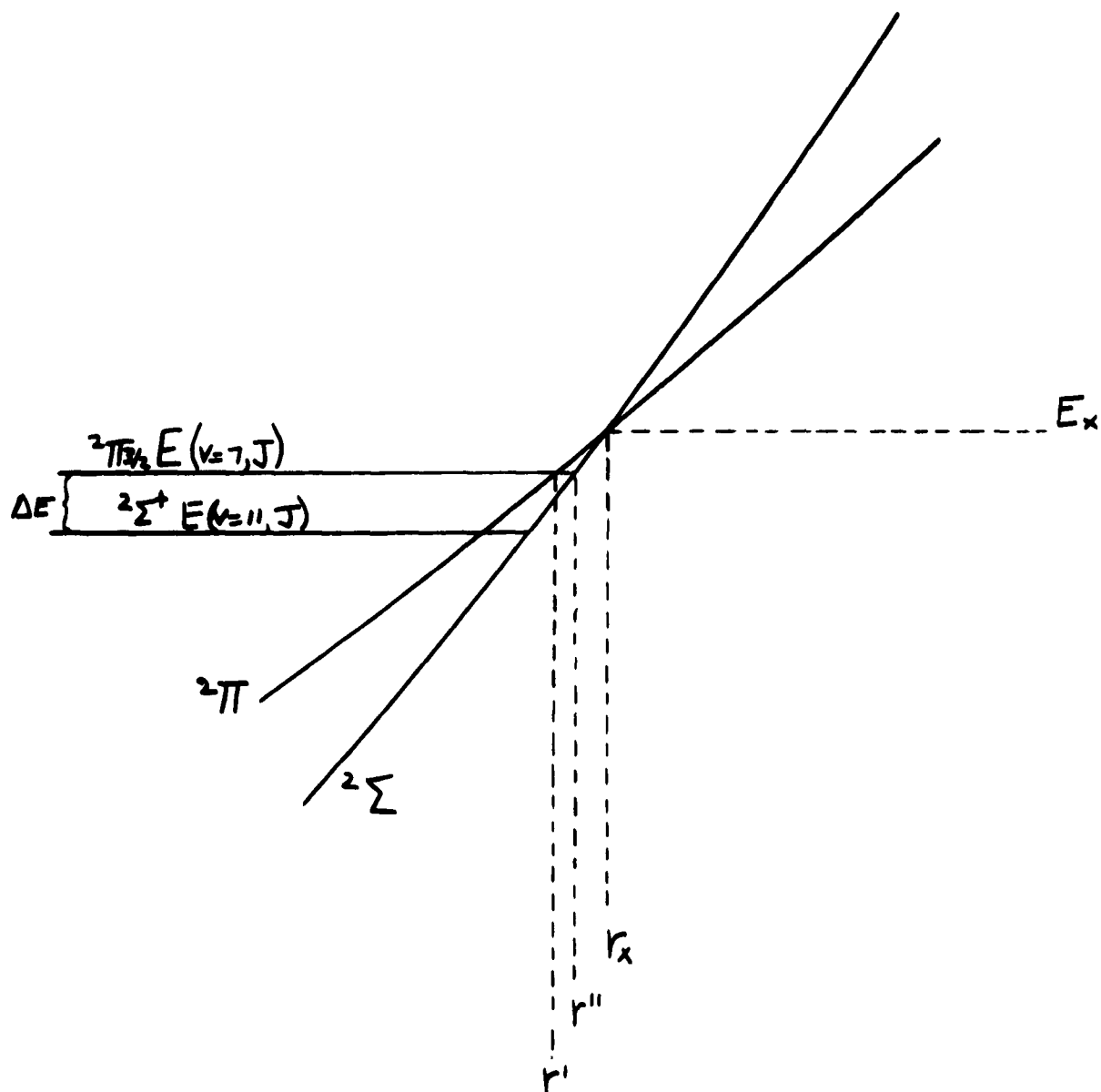


Table I. Potential Energy Curves for Different Electronic States of  $\text{CN}^a$ .

State	$T_e(\text{ev})$	$v$	$U(\text{cm}^{-1})$	$r_{\min}$	$r_{\max}$	$U(\text{ev})$	$U+T_e(\text{ev})$
$X^2\Sigma^+$	0	0	1031.2	1.1237	1.2244	0.1278	0.1278
		1	3073.6	1.0923	1.2676	0.3811	0.3811
		2	5089.7	1.0722	1.2997	0.6310	0.6310
		3	7079.5	1.0566	1.3274	0.8777	0.8777
		4	9042.8	1.0438	1.3525	1.1211	1.1211
		5	10980	1.0327	1.3760	1.3613	1.3613
		6	12890	1.0230	1.3984	1.5981	1.5981
		7	14775	1.0143	1.4198	1.8317	1.8317
		8	16632	1.0063	1.4406	2.0620	2.0620
		9	18463	0.9991	1.4610	2.2890	2.2890
		10	20267	0.9924	1.4809	2.5127	2.5127
		11	22045	0.9861	1.5005	2.7330	2.7330
		12	23797	0.9803	1.5200	2.9503	2.9503
		13	25520	0.9749	1.5393	3.1639	3.1639
		14	27217	0.9696	1.5583	3.3743	3.3743
		15	28887	0.9648	1.5774	3.5813	3.5813
		16	30530	0.9602	1.5964	3.7850	3.7850
		17	32146	0.9558	1.6153	3.9853	3.9853
$A^2\Pi_{3/2}(J=3/2)$	1.14332	18	33734	0.9516	1.6343	4.1823	4.1823
		0	903.99	1.1827	1.2900	0.1121	1.2554
		1	2691.1	1.1482	1.3354	0.3336	1.4770
		2	4452.9	1.1269	1.3701	0.5521	1.6954
		3	6189.4	1.1105	1.4001	0.7673	1.9107
		4	7900.4	1.0969	1.4273	0.9795	2.1228
		5	9585.9	1.0852	1.4529	1.1884	2.3318
		6	11245	1.0749	1.4773	1.3942	2.5375
		7	12880	1.0657	1.5007	1.5968	2.7401
		8	14487	1.0573	1.5236	1.7960	2.9393
		9	16070	1.0497	1.5459	1.9923	3.1356
		10	17627	1.0426	1.5679	2.1853	3.3286
		11	19158	1.0360	1.5896	2.3751	3.5184
		12	20663	1.0298	1.6111	2.5617	3.7051
		13	22142	1.0240	1.6325	2.7451	3.8884

Table I. Continued.

State	T <sub>0</sub> (ev)	v	U(cm <sup>-1</sup> )	r <sub>min</sub>	r <sub>max</sub>	U (ev)	U+T <sub>0</sub> (ev)
$\Lambda^2\Pi_{3/2}(J=3/2)$	1.14959	14	23594	1.0186	1.6538	2.9254	4.0687
		15	25021	1.0134	1.6750	3.1020	4.2454
		16	26422	1.0083	1.6960	3.2757	4.4190
		17	27795	1.0038	1.7175	3.4460	4.5893
		18	29142	0.9994	1.7388	3.6130	4.7563
$\Lambda^2\Pi_{1/2}(J=1/2)$		0	903.99	1.1816	1.2891	0.1121	1.2617
		1	2691.1	1.1484	1.3356	0.3336	1.4832
		2	4452.9	1.1272	1.3704	0.5521	1.7017
		3	6189.4	1.1109	1.4006	0.7673	1.9169
		4	7900.4	1.0975	1.4280	0.9795	2.1291
		5	9585.9	1.0860	1.4537	1.1884	2.3380
		6	11245	1.0759	1.4783	1.3942	2.5438
		7	12880	1.0668	1.5019	1.5968	2.7464
		8	14487	1.0587	1.5249	1.7960	2.9456
		9	16070	1.0512	1.5475	1.9923	3.1419
		10	17627	1.0443	1.5696	2.1853	3.3349
		11	19158	1.0379	1.5916	2.3751	3.5247
		12	20663	1.0319	1.6133	2.5617	3.7113
13	22142	1.0263	1.6348	2.7451	3.8947		
$B^2\Sigma^+$	3.1927	14	23594	1.0211	1.6563	2.9254	4.0750
		15	25021	1.0161	1.6778	3.1020	4.2516
		16	26422	1.0115	1.6992	3.2757	4.4253
		17	27795	1.0070	1.7207	3.4460	4.5956
		18	29142	1.0028	1.7423	3.6130	4.7626
		0	1077	1.104	1.203	0.1335	3.3262
		1	3200	1.074	1.246	0.3968	3.5895
		2	5284	1.055	1.279	0.6551	3.8478
		3	7325	1.040	1.307	0.9081	4.1008
		4	9321	1.027	1.333	1.1556	4.3483
5		11269	1.016	1.358	1.3971	4.5898	
6		13167	1.007	1.383	1.6324	4.8251	

Table I. Continued

State	$T_e(\text{ev})$	$v$	$U(\text{cm}^{-1})$	$r_{\min}$	$r_{\max}$	$U(\text{ev})$	$U+T_e(\text{ev})$
$B^2\Sigma^+$	3.1927	7	15011	0.999	1.407	1.8611	5.0538
		8	16799	0.992	1.432	2.0827	5.2753
		9	18527	0.986	1.457	2.2969	5.4896
		10	20192	0.980	1.483	2.5034	5.6961
		11	21795	0.974	1.509	2.7021	5.8948
		12	23338	0.970	1.535	2.8933	6.0860
		13	24821	0.965	1.562	3.0773	6.2699
		14	26249	0.961	1.589	3.2542	6.4469
		15	27623	0.957	1.617	3.4247	6.6173
		16	28948	0.953	1.644	3.5889	6.7816
		17	30228	0.950	1.672	3.7475	6.9402
		18	31464	0.946	1.701	3.9008	7.0934
$D^2\Pi_1$	6.7550	0	500.1	1.431	1.576	0.06201	6.8170
		1	1487	1.386	1.639	0.1844	6.9394
		2	2457	1.358	1.686	0.3046	7.0596
		3	3409	1.336	1.727	0.4226	7.1776
$J^2\Delta_1$	8.0902	0	557.4	1.351	1.488	0.06910	8.1593
		1	1651	1.310	1.550	0.2047	8.2949
		2	2719	1.285	1.598	0.3370	8.4272
		3	3760	1.266	1.640	0.4661	8.5563
		4	4777	1.250	1.679	0.5922	8.6824

<sup>a</sup> Note that the potential curve has been calculated for the  $J = 3/2$  and  $J = 1/2$  rotational levels of the  $^2\Pi_{3/2}$  and  $^2\Pi_{1/2}$  states respectively. These are the lowest possible  $J$  values.<sup>2</sup>



Table II. Significant Energy and Distance Points for Discussion of Rotational Perturbations in the  $^2\Pi_{3/2}$  and  $^2\Sigma^+$  States.<sup>a</sup>

J	$^2\Pi_{3/2}$ $E(v=7, J) \text{ cm}^{-1}$	$\Delta E (\text{cm}^{-1})$	$r' (\text{\AA})$	$r'' (\text{\AA})$	$r_x (\text{\AA})$	$E_x (\text{cm}^{-1})$
10 1/2	22,283	+ 9	1.5014	1.5017	1.5027	22,370
12 1/2	22,357	+ 4	1.5017	1.5020	1.5027	22,424
13 1/2	22,399	- 2	1.5019	1.5021	1.5027	22,452
14 1/2	22,444	- 7	1.5021	1.5022	1.5028	22,492
15 1/2	22,492	-14	1.5023	1.5024	1.5028	22,528
16 1/2	22,543	-20	1.5025	1.5026	1.5028	22,570
17 1/2	22,597	-27	1.5027	1.5027	1.5029	22,612
18 1/2	22,655	-31	1.5029	1.5029	1.5029	22,655

<sup>a</sup> Refer to Fig. 3 for explanation of symbols.

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